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The Strength of Chaos: accurate simulation of resonant electron scattering by many-electron ions and atoms in the presence of quantum chaos

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Abstract: The primarily goal of the project was to obtain benchmark cross sections for a complex quantum collision system that is electron scattering on molecular hydrogen. Such collision systems are ubiquitous in the universe, but are also prototypes of even more complex collision systems, such as those involving biologically relevant molecules, which may be described using a quantum chaotic approach.

Introduction: Electron collisions with atomic and molecular targets are ubiquitous all around us. There is no shortage of applications that are advanced by a quantitative understanding of such collisions, and include lighting, astrophysics, fusion energy through to cancer imaging and therapy. During the last two decades there has been immense progress in the field of electron scattering on relatively simple, quasi one-electron and two-electron, atomic and ionic targets [1]. The progress has been in both formal [2] and computational theory [3]. The next frontier is application to complex systems that have multi-electron atomic and molecular targets. The seed funding provided by this project was used to employ a postdoctoral researcher, Mark Zammit, for a period of six months to establish benchmark cross sections for the electron scattering on molecular hydrogen collision system. He is currently continuing this work with Dr. James Colgan, in the Theoretical Physics Division, at the Los Alamos National Laboratory.

Theory: The underlying theoretical approach to collisions that we use is known as the Convergent Close-Coupling (CCC) method [4]. Briefly, it expands the target wave function in large complete Laguerre bases, and thereby provides a square-integrable representation of the target discrete and continuous spectra. The computational complexity grows rapidly with the number of particles involved, as each one requires extra three dimensions of freedom. Consequently, applications thus far include only targets well-modeled as one or two valence electrons above a relatively inert Hartree-Fock core. The extension to molecular systems is further complicated by the degrees of freedom for the nuclei. This is handled using the Born-Oppenheimer approximation, and an adiabatic approach is available if required.

Results and Discussion: The CCC approach for electron scattering on molecular hydrogen has been completed early in 2016, and applied to the calculation of total ionization cross sections. The results were extraordinary, yielding complete agreement with experiment over the entire energy range from threshold through to high energies where the Born approximation becomes valid. This is a critical test of the CCC method that no other theory can match, and has been published in the top technical physics journal, Physical Review Letters, see appendix.

List of Publications and Significant Collaborations that resulted from your AOARD supported project: In standard format showing authors, title, journal, issue, pages, and date,

a) papers published in peer-reviewed journals,

- Complete Solution of Electronic Excitation and Ionization in Electron-Hydrogen Molecule Scattering MC Zammit, JS Savage, DV Fursa, I Bray Physical Review Letters 116 (23), 233201 (2016)

b) papers published in non-peer-reviewed journals or in conference proceedings,
c) conference presentations,
d) manuscripts submitted but not yet published, and
e) provide a list any interactions with industry or with Air Force Research Laboratory scientists or significant collaborations that resulted from this work.

- Considerable interaction and forthcoming collaboration with Dr. James Colgan, Theoretical Physics Division, Los Alamos National Laboratory. Mark Zammit is now employed there.

References

[1] Electrons and photons colliding with atoms: development and application of the convergent close-coupling method, I Bray, DV Fursa, AS Kheifets, AT Stelbovics, Journal of Physics B: Atomic, Molecular and Optical Physics 35 (15), R117 (2002)
[2] Surface-integral formulation of scattering theory, AS Kadyrov, I Bray, AM Mukhamedzhanov, AT Stelbovics, Annals of Physics 324 (7), 1516-1546 (2009)
[3] Electron-and photon-impact atomic ionisation, I Bray, DV Fursa, AS Kadyrov, AT Stelbovics, AS Kheifets, AM Mukhamedzhanov, Physics Reports 520, 135—174 (2012)
[4] Convergent close-coupling calculations of electron-hydrogen scattering, I Bray, AT Stelbovics, Physical Review A 46 (11), 6995

Appendix
Physical Review Letter arising from this work follows